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Diffusion Model for Gas Replacement in an Isostructural CH4-CO2 Hydrate System

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Abstract

© 2017 American Chemical Society. Guest exchange in clathrates is a complex activated phenomenon of the guest-host cage interaction on the molecular-scale level. To model this process, we develop a mathematical description for the nonequilibrium binary permeation of guest molecules during gas replacement based on the microscopic "hole-in-cage-wall" diffusive mechanism. The transport of gas molecules is envisaged as a series of jumps between occupied and empty neighboring cages without any significant lattice restructuring in the bulk. The gas exchange itself is seen as two-stage swapping initiated by almost instantaneous formation of a mixed hydrate layer on the hydrate surface followed by a much slower permeation-controlled process. The model is constrained by and validated with available time-resolved neutron diffraction data of the isostructural CH 4 guest replacement by CO 2 in methane hydrate, a process of possible importance for the sequestration of CO 2 with concomitant recovery of CH 4 in marine gas hydrates. (Graph Presented).

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References

[1] Falenty, A.; Qin, J.; Salamatin, A. N.; Yang, L.; Kuhs, W. F. Fluid Composition and Kinetics of the in Situ Replacement in CH-CO Hydrate System J. Phys. Chem. C 2016, 120, 27159-27172 10.1021/acs.jpcc.6b09460

[2] Ota, M.; Abe, Y.; Watanabe, M.; Smith, R. L.; Inomata, H. Methane Recovery from Methane Hydrate Using Pressurized CO Fluid Phase Equilib. 2005, 228-229, 553-559 10.1016/j.fluid.2004.10.002

[3] Ota, M.; Morohashi, K.; Abe, Y.; Watanabe, M.; Smith, R. L., Jr.; Inomata, H. Replacement of CH in the Hydrate by Use of Liquid CO Energy Convers. Manage. 2005, 46, 1680-1691 10.1016/j.enconman.2004.10.002

[4] Schicks, J. M.; Luzi, M.; Beeskow-Strauch, B. The Conversion Process of Hydrocarbon Hydrates into CO Hydrates and Vice Versa: Thermodynamic Considerations J. Phys. Chem. A 2011, 115, 13324-13331 10.1021/jp109812v

[5] Zhou, X.; Fan, S.; Liang, D.; Du, J. Replacement of Methane from Quartz Sand-Bearing Hydrate with Carbon Dioxide-in-Water Emulsion Energy Fuels 2008, 22, 1759-1764 10.1021/ef700705y

[6] Boswell, R.; Schoderbek, D.; Collett, T. S.; Ohtsuki, S.; White, M.; Anderson, B. J. The Iġnik Sikumi Field Experiment, Alaska North Slope: Design, Operations, and Implications for CO-CH Exchange in Gas Hydrate Reservoirs Energy Fuels 2017, 31, 140-153 10.1021/acs.energyfuels.6b01909

[7] Schoderbek, D.; Boswell, R. Ignik Sikumi #1, Gas Hydrate Test Well, Successfully Installed on the Alaska North Slope Fire ice 2011, 1-5

[8] Jung, J. W.; Espinoza, D. N.; Santamarina, J. C. Properties and Phenomena Relevant to CH-CO Replacement in Hydrate-Bearing Sediments J. Geophys. Res. 2010, 115, B10102s 10.1029/2009JB000812

[9] Falenty, A.; Murshed, M. M.; Salamatin, A. N.; Kuhs, W. F. Gas Replacement in Clathrate Hydrates During CO Injection - Kinetics and Micro-Structural Mechanism. In Tenth ISOPE Ocean Mining and Gas Hydrates Symposium; The International Society of Offshore and Polar Engineers (ISOPE): Szczecin, Poland, September 22-26, 2013; pp 109-115.

[10] Koh, D. Y.; Kang, H.; Lee, J. W.; Park, Y.; Kim, S. J.; Lee, J.; Lee, J. Y.; Lee, H. Energy-Efficient Natural Gas Hydrate Production Using Gas Exchange Appl. Energy 2016, 162, 114-130 10.1016/j.apenergy.2015.10.082

[11] Dec, S. F. Surface Transformation of Methane-Ethane sI and sII Clathrate Hydrates J. Phys. Chem. C 2012, 116, 9660-9665 10.1021/jp301766y

[12] Liu, B.; Pan, H.; Wang, X.; Li, F.; Sun, C.; Chen, G. Evaluation of Different CH-CO Replacement Processes in Hydrate-Bearing Sediments by Measuring P-Wave Velocity Energies 2013, 6, 6242-6254 10.3390/en6126242

[13] Iwai, Y.; Nakamura, H.; Hirata, M. Molecular Dynamics Simulation of Replacement of Methane Hydrate with Carbon Dioxide Mol. Simul. 2012, 38, 481-490 10.1080/08927022.2011.647817

[14] Kvamme, B.; Qasim, M.; Baig, K.; Kivela, P. H.; Bauman, J. Hydrate Phase Transition Kinetics from Phase Field Theory with Implicit Hydrodynamics and Heat Transport Int. J. Greenhouse Gas Control 2014, 29, 263-278 10.1016/j.ijggc.2014.08.003

[15] Bai, D. S.; Zhang, X. R.; Chen, G. J.; Wang, W. C. Replacement Mechanism of Methane Hydrate with Carbon Dioxide from Microsecond Molecular Dynamics Simulations Energy Environ. Sci. 2012, 5, 7033-7041 10.1039/c2ee21189k

[16] Yuan, Q.; Sun, C. Y.; Yang, X.; Ma, P. C.; Ma, Z. W.; Liu, B.; Ma, Q. L.; Yang, L. Y.; Chen, G. J. Recovery of Methane from Hydrate Reservoir with Gaseous Carbon Dioxide Using a Three-Dimensional Middle-Size Reactor Energy 2012, 40, 47-58 10.1016/j.energy.2012.02.043

[17] Hirohama, S.; Shimoyama, Y.; Wakabayashi, A.; Tatsuta, S.; Nishida, N. Conversion of CH-Hydrate to CO-Hydrate in Liquid CO J. Chem. Eng. Jpn. 1996, 29, 1014-1020 10.1252/jcej.29.1014

[18] Liang, S.; Liang, D.; Wu, N.; Yi, L.; Hu, G. Molecular Mechanisms of Gas Diffusion in CO Hydrates J. Phys. Chem. C 2016, 120, 16298-16304 10.1021/acs.jpcc.6b03111

[19] Peters, B.; Zimmermann, N. E. R.; Beckham, G. T.; Tester, J. W.; Trout, B. L. Path Sampling Calculation of Methane Diffusivity in Natural Gas Hydrates from a Water-Vacancy Assisted Mechanism J. Am. Chem. Soc. 2008, 130, 17342-17350 10.1021/ja802014m

[20] Vidal-Vidal, A.; Perez-Rodriguez, M.; Pineiro, M. M. Direct Transition Mechanism for Molecular Diffusion in Gas Hydrates RSC Adv. 2016, 6, 1966-1972 10.1039/C5RA17867C

[21] Salamatin, A. N.; Falenty, A.; Hansen, T. C.; Kuhs, W. F. Guest Migration Revealed in CO Clathrate Hydrates Energy Fuels 2015, 29, 5681-5691 10.1021/acs.energyfuels.5b01217

[22] Falenty, A.; Salamatin, A. N.; Kuhs, W. F. Kinetics of CO-Hydrate Formation from Ice Powders: Data Summary and Modeling Extended to Low Temperatures J. Phys. Chem. C 2013, 117, 8443-8457 10.1021/jp310972b

[23] Kuhs, W. F.; Staykova, D. K.; Salamatin, A. N. Formation of Methane Hydrate from Polydisperse Ice Powders J. Phys. Chem. B 2006, 110, 13283-13295 10.1021/jp061060f

[24] Zhou, X.; Lin, F.; Liang, D. Multiscale Analysis on CH-CO Swapping Phenomenon Occurred in Hydrates J. Phys. Chem. C 2016, 120, 25668-25677 10.1021/acs.jpcc.6b07444

[25] Sloan, E. D.; Koh, C. A. Clathrate Hydrates of Natural Gases, 3rd ed.; CRC Press, Taylor & Francis Group: Boca Raton, FL, 2008.

[26] van der Waals, J. H.; Platteeuw, J. C. Clathrate Solutions Adv. Chem. Phys. 1958, 2, 1-57 10.1002/9780470143483.ch1

[27] Chazallon, B.; Kuhs, W. F. In Situ Structural Properties of N, O, and Air-Clathrates by Neutron Diffraction J. Chem. Phys. 2002, 117, 308-320 10.1063/1.1480861

[28] Murshed, M. M.; Schmidt, B. C.; Kuhs, W. F. Kinetics of Methane-Ethane Gas Replacement in Clathrate-Hydrates Studied by Time-Resolved Neutron Diffraction and Raman Spectroscopy J. Phys. Chem. A 2010, 114, 247-255 10.1021/jp908016j

[29] Hansen, T. C.; Falenty, A.; Kuhs, W. F. Lattice Constants and Expansivities of Gas Hydrates from 10 K up to the Stability Limit J. Chem. Phys. 2016, 144, 054301 10.1063/1.4940729

[30] Kang, H.; Ahn, Y. H.; Koh, D. Y.; Kim, S.; Park, J.; Lee, H. Optical Interpretation of the Chemical Process of CH-CO Exchange and Its Application to Gas Hydrate Production J. Phys. Chem. C 2015, 119, 21353-21357 10.1021/acs.jpcc.5b05827

[31] Glavatskiy, K. S.; Vlugt, T. J. H.; Kjelstrup, S. Toward a Possibility to Exchange CO and CH in sI Clathrate Hydrates J. Phys. Chem. B 2012, 116, 3745-3753 10.1021/jp2119586

[32] Ning, F. L.; Glavatskiy, K.; Ji, Z.; Kjelstrup, S.; Vlugt, T. J. H. Compressibility, Thermal Expansion Coefficient and Heat Capacity of CH and CO Hydrate Mixtures Using Molecular Dynamics Simulations Phys. Chem. Chem. Phys. 2015, 17, 2869-2883 10.1039/C4CP04212C

[33] Ida, T.; Endo, K.; Matsumoto, D.; Kato, N.; Mizuno, M.; Suzuki, Y.; Tadokoro, M. Dynamic and Static Behaviors of CH and CO in Small and Large Cavities of Hydrate J. Mol. Struct. 2013, 1032, 275-280 10.1016/j.molstruc.2012.10.015

[34] Wang, X.; Sang, D. K.; Chen, J.; Mi, J. G. Theoretical Insights into Nucleation of CO and CH Hydrates for CO Capture and Storage Phys. Chem. Chem. Phys. 2014, 16, 26929-26937 10.1039/C4CP03709J

[35] Salamatin, A. N.; Hondoh, T.; Uchida, T.; Lipenkov, V. Y. Post-Nucleation Conversion of an Air Bubble to Clathrate Air-Hydrate Crystal in Ice J. Cryst. Growth 1998, 193, 197-218 10.1016/S0022-0248(98)00488-6

[36] Demurov, A.; Radhakrishnan, R.; Trout, B. L. Computations of Diffusivities in Ice and CO Clathrate Hydrates via Molecular Dynamics and Monte Carlo Simulations J. Chem. Phys. 2002, 116, 702-709 10.1063/1.1425821

[37] Kirschgen, T. M.; Zeidler, M. D.; Geil, B.; Fujara, F. A Deuteron NMR Study of the Tetrahydrofuran Clathrate Hydrate - Part II: Coupling of Rotational and Translational Dynamics of Water Phys. Chem. Chem. Phys. 2003, 5, 5247-5252 10.1039/b212472f

[38] Buch, V.; Devlin, J. P.; Monreal, I. A.; Jagoda-Cwiklik, B.; Uras-Aytemiz, N.; Cwiklik, L. Clathrate Hydrates with Hydrogen-Bonding Guests Phys. Chem. Chem. Phys. 2009, 11, 10245-10265 10.1039/b911600c

[39] Lasaga, A. C. Kinetic Theory in the Earth Sciences; Princeton University Press: Princeton, NJ, 1998.

[40] Katchalsky, A.; Curran, P. F. Nonequilibrium Thermodynamics in Biophysics; Harvard University Press: Cambridge, MA, 1965; p 258.

[41] Ballard, A. L.; Sloan, E. D. The Next Generation of Hydrate Prediction - Part III. Gibbs Energy Minimization Formalism Fluid Phase Equilib. 2004, 218, 15-31 10.1016/j.fluid.2003.08.005

[42] Duan, Z. H.; Hu, J. W. A New Cubic Equation of State and Its Applications to the Modeling of Vapor-Liquid Equilibria and Volumetric Properties of Natural Fluids Geochim. Cosmochim. Acta 2004, 68, 2997-3009 10.1016/j.gca.2003.11.034

[43] Sujith, K. S.; Ramachandran, C. N. Carbon Dioxide Induced Bubble Formation in a CH-CO-HO Ternary System: A Molecular Dynamics Simulation Study Phys. Chem. Chem. Phys. 2016, 18, 3746-3754 10.1039/C5CP05623C

[44] Moridis, G. J.; Collett, T. S.; Pooladi-Darvish, M.; Hancock, S.; Santamarina, C.; Boswell, R.; Kneafsey, T.; Rutqvist, J.; Kowalsky, M. B.; Reagan, M. T. et al. Challenges, Uncertainties, and Issues Facing Gas Production from Gas-Hydrate Deposits SPE Reserv. Eval. Eng. 2011, 14, 76-112 10.2118/131792-PA

[45] Moridis, G. J.; Collett, T. S.; Boswell, R.; Kurihara, M.; Reagan, M. T.; Koh, C.; Sloan, E. D. Toward Production from Gas Hydrates: Current Status, Assessment of Resources, and Simulation-Based Evaluation of Technology and Potential SPE Reserv. Eval. Eng. 2009, 12, 745-771 10.2118/114163-PA

[46] Espinoza, D. N.; Santamarina, J. C. P-Wave Monitoring of Hydrate-Bearing Sand During CH-CO Replacement Int. J. Greenhouse Gas Control 2011, 5, 1031-1038 10.1016/j.ijggc.2011.02.006

[47] Wang, X. H.; Li, F. G.; Xu, Y. X.; Sun, C. Y.; Pan, H.; Liu, B.; Yang, L. Y.; Chen, G. J.; Li, Q. P. Elastic Properties of Hydrate-Bearing Sandy Sediment During CH-CO Replacement Energy Convers. Manage. 2015, 99, 274-281 10.1016/j.enconman.2015.04.032

[48] Lo, H.; Lee, M.-T.; Lin, S.-T. Water Vacancy Driven Diffusion in Clathrate Hydrates: Molecular Dynamics Simulation Study J. Phys. Chem. C 2017, 121, 8280-8289 10.1021/acs.jpcc.7b00853

[49] Chandler, D. Interfaces and the Driving Force of Hydrophobic Assembly Nature 2005, 437, 640-647 10.1038/nature04162

[50] Chaouachi, M.; Falenty, A.; Sell, K.; Enzmann, F.; Kersten, M.; Haberthür, D.; Kuhs, W. F. Microstructural Evolution of Gas Hydrates in Sedimentary Matrices Observed with Synchrotron X-Ray Computed Tomographic Microscopy Geochem., Geophys., Geosyst. 2015, 16, 1711-1722 10.1002/2015GC005811

[51] Yang, L.; Falenty, A.; Chaouachi, M.; Haberthür, D.; Kuhs, W. F. Synchrotron X-Ray Computed Microtomography Study on Gas Hydrate Decomposition in a Sedimentary Matrix Geochem., Geophys., Geosyst. 2016, 17, 3717-3732 10.1002/2016GC006521

[52] Uchida, T.; Yamazaki, K.; Gohara, K. Gas Nanobubbles as Nucleation Acceleration in the Gas-Hydrate Memory Effect J. Phys. Chem. C 2016, 120, 26620-26629 10.1021/acs.jpcc.6b07995

[53] Chaouachi, M.; Neher, S. H.; Falenty, A.; Kuhs, W. F. Time Resolved Coarsening of Clathrate Crystals: The Case of Gas Hydrates Cryst. Growth Des. 2017, 17, 2458-2472 10.1021/acs.cgd.6b01875

[54] Wu, J. Y.; Ning, F. L.; Trinh, T. T.; Kjelstrup, S.; Vlugt, T. J. H.; He, J. Y.; Skallerud, B. H.; Zhang, Z. L. Mechanical Instability of Monocrystalline and Polycrystalline Methane Hydrates Nat. Commun. 2015, 6, 8743 10.1038/ncomms9743

[55] Uras-Aytemiz, N.; Cwiklik, L.; Devlin, J. P. Tracking All-Vapor Instant Gas-Hydrate Formation and Guest Molecule Populations: A Possible Probe for Molecules Trapped in Water Nanodroplets J. Chem. Phys. 2012, 137, 204501 10.1063/1.4767370

[56] Devlin, J. P.; Buch, V. Evidence for the Surface Origin of Point Defects in Ice: Control of Interior Proton Activity by Adsorbates J. Chem. Phys. 2007, 127, 091101 10.1063/1.2768517

[57] Klapp, S. A.; Hemes, S.; Klein, H.; Bohrmann, G.; MacDonald, I.; Kuhs, W. F. Grain Size Measurements of Natural Gas Hydrates Mar. Geol. 2010, 274, 85-94 10.1016/j.margeo.2010.03.007

[58] Rempel, A. W. A Model for the Diffusive Growth of Hydrate Saturation Anomalies in Layered Sediments J. Geophys. Res. 2011, 116, B10105 10.1029/2011JB008484

[59] Kvamme, B. Thermodynamic Limitations of the CO/N Mixture Injected into CH Hydrate in the Ignik Sikumi Field Trial J. Chem. Eng. Data 2016, 61, 1280-1295 10.1021/acs.jced.5b00930